

This listing of claims will replace all prior versions, and listings of claims in the application:

Listing of Claims:

1-64. Canceled.

65. (Amended) A computer implemented process for producing a representation of a spectrum for a hypothetical solution containing a compound, for use in determining the composition of a test sample, the process comprising:

producing a position value for at least one peak of a reference spectrum as a function of a measured condition of the test sample, and a property of said at least one peak in a base reference spectrum.

66. (Original) The process of claim 65 wherein producing a position value comprises interpolating said position value from position values associated with base reference spectra associated with a condition nearest to said measured condition.

67. (Original) The process of claim 65 wherein producing a position value comprises calculating said position value as a function of pH of said sample.

68. (Original) The process of claim 65 wherein producing a position value comprises producing said position value by addressing a lookup table of position values with a measured condition value representing said condition of said sample.

69. (Original) The process of claim 65 further comprising accessing a pre defined record specifying peaks in a reference spectrum and adjusting a position value in said record, said position value being said position value of said at least one peak.

70. (Original) The process of claim 69 wherein adjusting comprises locating a condition value dependent function in said pre defined record, producing said position value from said function and associating said position value with said pre defined record.

71. (Original) The process of claim 70 wherein associating comprises storing said position value in said pre defined record.

72. (Original) The process of claim 69 wherein adjusting comprises locating in said pre defined record a link to a lookup table specifying peak positions for various conditions and retrieving said position value from said lookup table and associating said position value with said pre defined record.

73. (Original) The process of claim 72 wherein associating comprises storing said position value in said pre defined record.

74. (Original) A computer readable medium for providing computer readable instructions for causing a processor circuit to produce a representation of a spectrum for a hypothetical solution containing a compound, for use in determining the composition of a test sample, the instructions comprising:

a set of codes for directing the processor circuit to produce a position value for at least one peak of a reference spectrum as a function of a measured condition of the test sample, and a property of said at least one peak in a base reference spectrum.

75. (Original) A signal operable to cause a processor circuit to produce a representation of a spectrum for a hypothetical solution containing a compound, for use in determining the composition of a test sample, the signal comprising a signal segment comprising codes operable to cause the processor circuit to produce a position value for at least one peak of a reference spectrum as a function of a measured condition of the test sample, and a property of said at least one peak in a base reference spectrum.

76. (Original) An apparatus for producing a representation of a spectrum for a hypothetical solution containing a compound, for use in determining the composition of a test sample, the apparatus comprising a processor circuit programmed to produce a position value for at least one peak of a reference spectrum as a function of a measured condition of the test sample, and a property of said at least one peak in a base reference spectrum.

77. (Original) An apparatus for producing a representation of a spectrum for a hypothetical solution containing a compound, for use in determining the composition of a test sample, the apparatus comprising:

means for receiving a measured condition value representing a condition of the test sample;

means for receiving a representation of a position of at least one peak in a base reference spectrum; and

means for producing a position value for at least one peak of a derived reference spectrum as a function of said measured condition value of the test sample, and the position of said at least one peak in a base reference spectrum.